## Dislocation Formation During Growth of Semiconductor Crystals

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In the ongoing efforts to produce higher quality semiconductor materials, there is a continuous search for ways to consistently make materials with fewer defects. Thus, improvements in the understanding of how and why defects form would be extremely beneficial. This research examined one of the factors believed to affect dislocation formation during the growth of semiconductor crystals.

During directional solidification of semiconductor crystals, dislocations propagate from the existing crystal to the growing crystal at the melt/solid interface and from the solid/crucible surface into the growing crystal. Modeling efforts have shown that the interaction between the crucible wall and the sample in the region of the melt/solid interface has a significant effect on dislocation formation. Previous experimentation in microgravity has shown that when the melt is not in contact with the wall of the crucible, the resulting crystal will have a lower dislocation density. It is hypothesized that the increased ability of the crystal to relieve stresses is responsible for the lower dislocation density. The research done under the current ground-based funding will help to prepare for future space flight investigations of the effect of forced contact versus detachment of the melt from the crucible wall on dislocation structure during directional solidification of semiconductor crystals. The current research also involved characterization of a spring that would be necessary for maintaining melt/crucible contact during future flight experimentation.

Traditionally, solidification experiments have been done in microgravity due to the significant reduction in buoyancy driven convection that can be achieved in this environment. In this research, it is the desire to form a free surface in the region of the melt/solid interface that necessitates a microgravity environment. In a 1-g environment, the hydrostatic pressure of the melt is sufficient to keep the melt in contact with the wall of the crucible during vertical Bridgman crystal growth. In microgravity, the pressure on the melt is reduced or eliminated depending on the orientation of the acceleration vector. This can lead to the formation of a free surface on the melt. Ideally, this free surface will form in the region of the melt-solid interface and thus provide a crystal in which to study the effect of the free surface on defect formation.

Microgravity is necessary to investigate the case of a melt detached from the crucible wall. If this program is selected for flight in the future, two types of experiments are proposed to be done in microgravity. One type of experiments would employ a spring to prevent the formation of a free surface on the melt and one would, hopefully, result in the formation of a free surface at the solidification interface.

PBN (pyrolytic boron nitride) leaf springs have been used in previous GaAs crystal growth experiments in microgravity (GTE Get Away Special and United States Microgravity Laboratory-1 and -2) to insure that the melt remained in contact with the container. As part of the current ground-based program, a statistically sound design of experiments was

developed for determining the spring constant of a stack of PBN leaf springs. A fully quadratic empirical model will be developed in terms of the leaf radius, width, height, and the number of leaves in the stack. This will enable the prediction of the force applied on the melt from a stack of leaf springs of a given size. In addition, a theoretical model will be compared to the empirical model.

Gallium-doped germanium (Ga/Ge) crystals are being grown using the vertical Bridgman technique. Crystals grown in contact with a PBN crucible and grown with a boric oxide encapsulant are being examined to determine the effect of the encapsulant on the resulting dislocation density. It was hypothesized that the use of an encapsulant would allow the crystal to relieve stresses similarly to the case of a detached melt.

Full-scale numerical simulations of the experiment are an integral part of the proposed work. The full GTE/GAS furnace/ampoule/charge assembly will be included in a finite element numerical model. Time dependent simulations will track the entire experiment from cold start to final cool down, allowing the determination of the solidification thermal history in the growing crystal under the different growth scenarios. The time dependent thermal history will then form the input database for subsequent calculations of the stress field. Using a viscoplastic Haasan-Alexander full crystallographic constitutive model with different boundary conditions reflecting the crystal detachment/attachment to the crucible, the dislocation multiplication and resolved stresses in each individual crystallographic slip system will be computed.

The knowledge gained from the current ground-based experiments will be useful when ampoules are designed for Space Station-era experiments in microgravity. In addition, the ability to predict the force of a stack of PBN leaf springs makes the potential use of this type of spring much greater for many other applications. The knowledge gained from future flight experiments combined with a vigorous modeling effort is expected to contribute significantly to the understanding of how and why dislocations form during the growth of semiconductors. This information will be useful to ground-based research efforts that are trying to reduce the number of defects in semiconductor crystals.